RESEARCH ARTICLE

Performance of turbulence models for dense gas release in computational fluid dynamics

The prediction of temporal and spatial concentration profiles of gas cloud is of great importance in safety issues. Existing models for predicting dense gases release are used for flat plates, and they cannot usually involve the complex environments, hence in this article, computational fluid dynamics have been used for prediction of dense gases behavior. The selection of turbulence model shows its significance in the results of computational fluid dynamics. In order to select the best turbulence model, the models of k–ε and k–ω have been studied. Experimental data of the test no. 26 of Thorney Island Series data have been extracted. The results show that k–ε realizable model is closest to the experimental data. This model has the closest and most appropriate prediction of the spatial and temporal profile. The model is also able to predict the phenomenon of gravity slumping associated with dense gas dispersion.

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INTRODUCTION

Chemical manufacturing and use enterprises often have strong concerns regarding gas releases from their processes particularly during emergencies. Current, commonly used models such as HEGADAS,[1] SLAB,[2] HGSYSTEM,[3] ALOHA,[4] SCIPUFF[5] and others can have difficulty in complex metrological environments. Computational fluid dynamics (CFD) can be an appropriate tool for modeling gas releases in a 3-dimensional environment.[6]

Kisa and Jelemensky modeled liquefied ammonia dispersion using Fluent version 6.2, which is a CFD approach.[7] Their results were compared with FLADIS data obtained by Nielsen et al.[8] Moulilleau and Champassith modeled atmospheric gas releases using fire dynamics simulation, also a CFD process.[9] Pontigga et al. modeled sulfur dioxide gas dispersion using CFD techniques and compared the results with experimental data.[10]

Tang et al.[11] evaluated the accuracy of CFD in modeling gases dispersion in the atmosphere, they have modeled wind tests which once were done in 1958 with the use of CFD, and compared the results with experimental data. And they conclude that k–ε model is suitable to studying the dispersion in the atmosphere.

Hanjalic and Kenjeres investigated the pollution over a middle sized town located in a mountain area.[12] This study was done in a winter day without wind in an inversion condition. The heat generated in the city was considered and dispersion of pollution was studied in the city for two days. Some studies have compared dispersion models with the results of CFD, for example, Riddle et al.[13] have compared the results from the CFD with results of results of Atmospheric Dispersion Modeling System (ADMS) model.

Many software packages exist for CFD modeling. We have chosen FLUENT for this study. There are many models available. Selecting a model which correctly predicts gas release behavior is important. We selected k–ε and k–ω models to more correctly predict turbulence modeling and extracted experimental data from the experiment no. 26 of the Thorney Island Heavy Gas Dispersion Trials.[14] The k–ε standard,[15] k–ε RNG,[16] k–ε realizable[17] and k–ω standard[18] models are two equation models and are frequently used for incompressible, low-speed flows in isotropic turbulence.[19]

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DESCRIPTION OF THE EXPERIMENTAL MODEL

In the Thorney Island experiment number 26, a 14 m (diameter) × 13 m (high) tank containing a gas mixture of 31.6% Freon-12 (w/w) in nitrogen is placed 50 m from a 9-m cubic obstacle is released for 1.5 s. The release is characterized in Table 1.

The test environment is a rectangular parallelepiped of 200 m (length) × 150 m (width) × 50 m (height). The domain was carefully meshed in a manner to maximize the detailing of the regions of importance. For example, in order to consider pressure and velocity gradients at the boundaries, a “fine” mesh was used near the ground and obstacle. In regions of lesser importance, the mesh is coarser. The total mesh contained 461, 638 cells.

Figure 1 shows the geometry of the floor meshes and boundary conditions.

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Table 1. The Amount of Release and Other Release Characteristics.

Experiment No.	Released Gaseous Mixture Density Relative to Air	Total Released Volume (m^3)	Total Released Mass (kg)	Mass and Flow Rate (kg/s)
26	2	1970	4767	3187

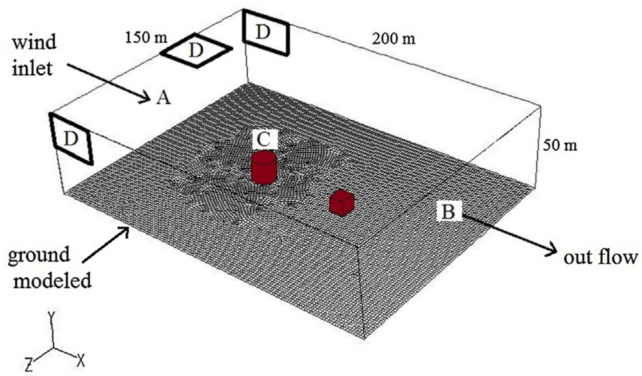

Figure 1. Simulated geometry for data validation.

There are four boundary conditions (A–D in Figure 1) specified for this modeling. These four boundary conditions are:

1. Velocity inlet boundary condition: to obtain a profile of wind speed, Eq. (1) is used:

$$u_y = u_0 \times \left(\frac{y}{y_0}\right)^{\lambda} \tag{1}$$

   where u_y is the wind speed at height (y-axis) and u_0 is the reported speed at height "y." In the case studied, $u_0 = 1.9$ m/s and $y = 10$ m. The test is conducted in "Class B" atmospheric conditions as defined in Ref. 15, which makes $\lambda = 0.07$.[20]
2. Outflow boundary condition: since it is not clear the rate and pressure's flow at the exit boundary (right wall), the right boundary is defined as outflow. This boundary condition is applied on the assumption that air and Freon-12/nitrogen mixture are incompressible.
3. Mass flow inlet boundary condition: gas emits from the upper surface of the cylinder to the enclosure, and the mass flow inlet boundary condition is accordance with a rate of 3178 kg/s perpendicular to the release screen within the mass fraction of 68.4% N_2 and 31.6% Freon-12.
4. Wall boundary condition: this condition has been considered for all walls and the floor, in this boundary condition the velocity and concentration gradients is zero. This assumption is supported by the fact that these boundaries are at a great distance from the region and the gradients would be nearly zero there.

In order to evaluate the accuracy and exactness of the turbulence models, k–ε and k–ω models are considered, to determine the accuracy and exactness of these models and to choose the best model for dense gases release.

The computer used in this modeling has a processor with 2.4 GHz Intel® core i3 and memory of 3 GB.

RESULTS

In order to study the gas release, the energy, mass and momentum equations have been solved in the specified space. To obtain initial and steady state values for the simulation a wind velocity profile was developed without a release. The wind velocity profile is shown in Figure 2. We see that there a vortex may form behind the barrier which would cause gas accumulation in that area (Figure 3).

For the present case, the problem was initially solved in steady state to obtain initial values for the transient simulation (Figure 2). After obtaining steady state wind at the start of the experiment the dispersion was

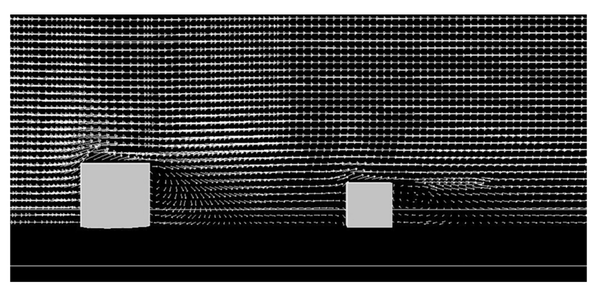

Figure 2. Wind profile in space results of k–ε realizable model.

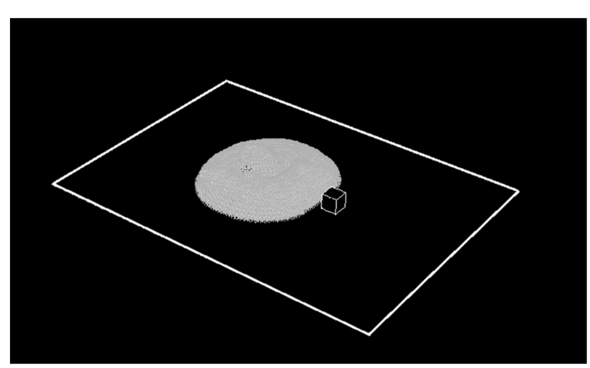

Figure 3. Gas cloud after 10 s of release results of k–ε realizable model.

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